Title: **Using Godunov's Two-Sided Sturm Sequences to Accurately Compute Singular Vectors of Bidiagonal Matrices**

Author(s): A.M. Matsekh and E.P. Shurina

Submitted to:

http://lib-www.lanl.gov/cgi-bin/getfile?00937093.pdf

Using Godunov's Two-Sided Sturm Sequences to Accurately Compute Singular Vectors of Bidiagonal Matrices.

A.M. Matsekh[*][†] *E.P. Shurina*[‡]

1 Introduction

We present a hybrid scheme for computing singular vectors of bidiagonal matrices based on Godunov's two-sided Sturm sequence method [1] and Inverse Iteration [2]. This scheme is applied to the equivalent tridiagonal symmetric eigenvalue problem with corresponding matrix in the Golub-Kahan form. Two-sided Sturm sequences and the underlining theory were introduced in early 80's by S.K.Godunov who showed that provably accurate eigenvectors can be computed from two-sided Sturm sequences in only $O(n)$ floating operations per an eigenvector from the corresponding two-sided Sturm sequence. This is equivalent to determining and eliminating redundant equation from the homogeneous underdetermined linear system $(A - \lambda I)x = 0$. This was the first provably accurate solution to the Wilkinson's problem [2], [3]. Unfortunately in finite precision Godunov's eigenvectors deliver residuals that are a few orders of magnitude larger than residuals of eigenvectors

[*]matsekh@lanl.gov

[†]Institute of Computational Technologies, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, Russian Federation. Currently: Computer and Computational Sciences Division, Los Alamos National Laboratory, Los Alamos, NM, USA.

[‡]Applied Mathematics Department, Novosibirsk State Technical University, Novosibirsk, Russian Federation.

computed with some implementations of Inverse Iteration. To improve accuracy of eigenvectors and singular vectors computed using Godunov's method, we developed a hybrid algorithm which we call Godunov-Inverse Iteration. The computational scheme that we use to find singular vectors of bidiagonal matrices using this hybrid method can be described as follows. We use a version of bisection method based on the classical, or, in Godunov's terminology, one-sided Sturm-sequences, to find the smallest machine representable intervals that contain eigenvalues of the Golub-Kahan form with high guaranteed accuracy, followed by Godunov's method to find eigenvector approximations of the Golub-Kahan matrix. We then apply one or two steps of Inverse Iteration with reorthogonalization with a special choice of shift and selective reorthogonalization to iteratively improve the computed eigenvectors. The resulting eigenvectors contain interlacing components of the corresponding left and right singular vectors of the original matrix. Eigenvectors and singular vectors computed using Godunov–Inverse Iteration do not suffer from the loss of accuracy and orthogonality characteristic of finite precision implementations of Godunov's method, and typically requires only one iteration step to obtain singular vectors that satisfy original problem to higher accuracy than Inverse Iteration which can take up to six iteration steps to converge. In addition convergence of the Inverse Iteration is not guaranteed, while Godunov-Inverse Iteration inherits guaranteed nature of Godunov's algorithm.

2   Singular value decomposition

An arbitrary matrix $A \in R^{p \times m}$ can be reduced to an equivalent form

$$\widetilde{D} = P^* A Q$$

where $P \in R^{p \times p}$ and $Q \in R^{m \times m}$ are orthogonal, and nonzero part $D \in R^{n \times n}$, $n = \min\{p, m\}$ of the matrix $\widetilde{D} \in R^{p \times m}$ is a bidiagonal matrix [4]. Without loss of generality we can assume that D is an upper bidiagonal matrix of the form:

$$D = \begin{pmatrix} c_0 & a_0 & & & \\ & c_1 & a_1 & & \\ & & \ddots & \ddots & \\ & & & c_{n-2} & a_{n-2} \\ & & & & c_{n-1} \end{pmatrix}. \tag{1}$$

Singular value decomposition

$$D = X \Sigma Y^*$$

factors matrix $D \in R^{n \times n}$ into the product of orthogonal matrices $X \in R^{n \times n}$ and $Y \in R^{n \times n}$ and diagonal matrix Σ with singular values σ_i, $i = 1, 2, \ldots, n$ on its main diagonal. Singular values and singular vectors of the matrix D can be found by solving symmetric eigenvalue problem with the matrix D in the Jordan-Wielandt form [5], [6]:

$$J = \begin{bmatrix} 0 & D \\ D^* & 0 \end{bmatrix}.$$

Spectrum of the matrix J contains singular values of the matrix D:

$$\lambda(J) = \{\sigma(D)\} \cup \{-\sigma(D)\}.$$

A more economical approach to finding singular values of the matrix D from a matrix permutationally equivalent to the matrix J was introduced by Golub and Kahan [7]. In this approach J is transformed to the permutationally equivalent tridiagonal symmetric matrix G with zeros on the main diagonal which Fernando [5] proposed to call the Golub-Kahan form:

$$
G =
\begin{pmatrix}
0 & c_0 & & & & & \\
c_0 & 0 & a_0 & & & & \\
& a_0 & 0 & c_1 & & & \\
& & c_1 & \ddots & \ddots & & \\
& & & \ddots & 0 & c_{n-1} & \\
& & & & c_{n-1} & 0 &
\end{pmatrix}.
\tag{2}
$$

Permutation is an orthogonal transformation, which means that it keeps spectral properties of the matrix J unchanged, that is:

$$\lambda(G) = \{\sigma(D)\} \cup \{-\sigma(D)\}.$$

Let Π be a permutation which transforms Jordan-Wielandt form of the bidiagonal matrix D to the corresponding Golub-Kahan form. When applied to the composite vector

$$w = \begin{pmatrix} v \\ u \end{pmatrix}$$

permutation P transforms w into the vector with interlacing components of u and v:

$$
x = \Pi \begin{pmatrix} v \\ u \end{pmatrix} = \Pi
\begin{pmatrix}
v_1 \\ \vdots \\ v_n \\ u_1 \\ \vdots \\ u_n
\end{pmatrix}
=
\begin{pmatrix}
v_1 \\ u_1 \\ v_2 \\ u_2 \\ \vdots \\ v_n \\ u_n
\end{pmatrix}.
\tag{3}
$$

If w is an eigenvector of the Jordan-Wielandt matrix $\widetilde{J}$, then

$$\Pi \widetilde{J} w = \Pi \widetilde{J} \Pi^* \Pi w = G \Pi w = G x,$$

which means that components of the left and right singular vectors v and u can be easily recovered from the eigenvectors of the corresponding Golub-Kahan matrix G using relationship (3).

3 Bisection method based on one-sided Sturm sequences

The accuracy of eigenvectors computed by Godunov's method strongly depends on the accuracy of the eigenintervals computed with the bisection method. Following Godunov [8] we implemented a finite precision variant of the Wilkinson's bisection algorithm [2] which uses Sturm sequences to find intervals (α_i, β_i) containing eigenvalues μ_i of the tridiagonal symmetric matrix G

$$G = \begin{pmatrix} d_0 & b_0 & & & \\ b_0 & d_1 & b_1 & & \\ & b_1 & \ddots & \ddots & \\ & & \ddots & \ddots & b_{n-2} \\ & & & b_{n-2} & d_{n-1} \end{pmatrix} \tag{4}$$

with guaranteed accuracy

$$|\beta_i - \alpha_i| \leq \epsilon_{mach}\, \mathfrak{F}(G), \ \ i = 1, \ldots, n,$$

where ϵ_{mach} is the unit roundoff error and $\mathfrak{F}(G)$ is some norm of the matrix G. We prefer Godunov's version of the bisection method [8] based on the use of Sturm sequences to the inertia based bisection method [5], as in our implementations Sturm sequences give slightly more accurate eigenvalue approximations. Sturm sequence of the tridiagonal symmetric matrix G (4) (or in Godunov's terminology one-sided Sturm sequence) is computed for an eigenvalue approximation λ as follows:

$$P_0(\lambda) = \begin{cases} |b_0|/(d_0 - \lambda), & b_0 \neq 0 \\[2mm] 1/(d_0 - \lambda), & b_0 = 0 \end{cases} \tag{5a}$$

$$P_k(\lambda) = \begin{cases} |b_k|/(d_k - \lambda - |b_{k-1}|)P_{k-1}(\lambda), & b_k \neq 0 \cap k < (n-1) \\[2mm] 1/(d_k - \lambda - |b_{k-1}|)P_{k-1}(\lambda), & b_k = 0 \cup k = (n-1), \end{cases}, \tag{5b}$$

where $k = 1, 3, \ldots, n-1$. Bisection method uses Sturm theorem which states that the number of nonpositive elements in the recurrence (5) coincides with the number of eigenvalues of the matrix G which are less than λ. In eigenvalue problems initial interval (β, α) is determined from Gershgorin circles. In singular value computations for the Golub-Kahan form we can give a more accurate estimate of the initial interval to be partitioned. Singular values of the bigiagonal matrix D (1) coincide with nonnegative eigenvalues of the corresponding Golub-Kahan matrix G (2). It should be noted that if none of the diagonal elements c_i, a_i, of the bidiagonal matrix D (1) is zero, than all singular values of the matrix D are positive [8]:

$$0 < \lambda_{n+1} < \lambda_{n+2} < \ldots < \lambda_{2n} < \mathfrak{M}(G),$$

where $\mathfrak{M}(G)$ is sometimes refereed to as Gershgorin norm of the matrix G and is computed as follows:

$$\mathfrak{M}(G) = \max \begin{cases} |d_0| + b_0| \\ \max\limits_{1 \leq i < n-1} |d_i| + |b_i| + |b_{i+1}| \\ |d_{n-1}| + |b_{n-1}| \end{cases}. \tag{6}$$

Upper bound Y of the initial bisection interval $[X, Y]$ can be chosen to be

$$Y = \mathfrak{M}(G),$$

while lower bound X can be determined as follows:

$$X = |c_0 c_1 \cdots c_{n-1}| / Y^{n-1}.$$

Obviously if numbers c_i, $i = 0 \ldots n$ are very small in floating point arithmetics X can get arbitrary small and as a result rounded to zero. In this case rescaling can be used to compute X. By letting $\lambda' = (X + Y)/2$ in the classical bisection method we can compute Sturm sequence for λ' and thus determine whether eigenvalue (singular value) λ belongs to $[X, \lambda')$, or $(\lambda', Y]$. We then set interval $[X, Y]$ to be either $[X, \lambda')$, or $(\lambda', Y]$. This process is repeated until the size of the interval $[X, Y]$ is comparable to the unit roundoff error ϵ_{mach}. Godunov's algorithm requires an interval version of the bisection method, in which instead of the eigenvalue approximation $\lambda' = (X + Y)/2$ eigeninterval $[\lambda' - \delta, \lambda' + \delta]$ is considered, and subintervals $[X, \lambda' - \delta)$, $(\lambda' + \delta, Y]$ are considered instead of the subintervals $[X, \lambda')$, $(\lambda', Y]$, and where δ is a small disturbance in the order ϵ_{mach}. In our implementation of Godunov's bisection algorithm unit roundoff ϵ_{mach} is an optimal choice of the parameter δ. We generally terminate this iteration when the following condition is satisfied [9]:

$$|\beta_i - \alpha_i| \leq \epsilon_{mach}(|\beta_i| + |\alpha_i|), \ i = 1, \ldots, n$$

or the number of iterations equals

$$t = [\log_2(\mathfrak{M}(G)/\epsilon_{mach})].$$

Indeed, the length of the largest initial bisection interval is $\mathfrak{M}(G)$ and after t bisection steps the length of the interval will be comparable to the unit roundoff ϵ_{mach}:

$$\mathfrak{M}(G)/2^t \simeq \epsilon_{mach}.$$

4 Godunov's method and Godunov–Inverse Iteration

Godunov's method [8], [1] was designed to compute eigenvectors of an unreduced symmetric tridiagonal matrix (4) in a floating point model that supports extended precision and directed rounding. Let (α_i, β_i) be an eigeninterval that is guaranteed to contain an eigenvalue $\mu_i(G)$ of the matrix G. Such an interval can be found by the bisection method with the accuracy [8]

$$|\beta_i - \alpha_i| \leq \mathfrak{c}(\gamma)\, \epsilon_{mach}\, \mathfrak{M}(G), \tag{7}$$

where $\mathfrak{c}(\gamma)$ is a constant that depends on the base of floating point exponent γ, and $\mathfrak{M}(G)$ is Gershrorin norm of the matrix G (6). Godunov derives left-sided Sturm sequence $P_k^+(\alpha_i)$ from the minors of the matrix $G - \alpha_i I$ [8]:

$$P_0^+(\alpha_i) = |b_0|/(d_0 - \alpha_i) \tag{8a}$$

$$P_k^+(\alpha_i) = |b_k|/(d_k - \alpha_i - |b_{k-1}|)P_{k-1}^+(\alpha_i) \tag{8b}$$

$$P_{n-1}^+(\alpha_i) = 1/(d_{n-1} - \alpha_i - |b_{n-2}|)P_{n-2}^+(\alpha_i) \tag{8c}$$

and the right-sided Sturm sequence $P_k^-(\beta_i)$ from the minors of the matrix $G - \beta_i I$ [8]:

$$P_{n-1}^-(\beta_i) = d_{n-1} - \beta_i \tag{9a}$$

$$P_k^-(\beta_i) = (d_k - \beta_i - |b_k|/P_{k+1}^-(\beta_i))/|b_{k-1}| \tag{9b}$$

$$P_0^-(\beta_i) = d_0 - \beta_i - |b_0|/P_1^-(\beta_i) \tag{9c}$$

Left-sided and right-sided Sturm sequences are then joint into the two-sided Sturm sequence

$$P_0(\mu_i), \ldots, P_{n-1}(\mu_i) \stackrel{\text{def}}{=} P_0^+(\alpha_i), \ldots P_l^+(\alpha_i), P_{l+1}^-(\beta_i), \ldots P_{n-1}^-(\beta_i). \tag{10}$$

Sequences (8) and (9) are joint at the index $l = l^+ = l^-$ which satisfies the following condition [8]:

$$(P_l^+(\alpha_i) - P_l^-(\beta_i))(1/P_{l+1}^-(\beta_i) - 1/P_{l+1}^+(\alpha_i)) \leq 0,$$

where l^+ be the number of nonpositive elements in the sequence $P_k^+(\alpha_i)$, $k = 0, \ldots, n - 1$, and $n - 1 - l^-$ is the number of nonnegative elements in the sequence $P_k^-(\beta_i)$, $k = n - 1, \ldots, 0$. Resulting two-sided Sturm sequence (10) is used to compute provably accurate eigenvector approximation u^i corresponding to the eigenvalue approximation $\mu_i(G) \in (\alpha_i, \beta_i)$ as follows:

$$u_0^i = 1 \text{ and } u_k^i = -u_{k-1}^i \text{sign}(b_{k-1})/P_{k-1}(\mu_i). \tag{11}$$

This computation requires only $O(n)$ operations per a normalized eigenvector. In finite precision eigenvectors constructed from the left-sided and the right-sided Sturm sequences for the same parameter λ are different, even though analytically they coincide. If matrix G (4) is a Golub-Kahan matrix, presence of zero elements on the main diagonal may result in nonnumeric values of the elements of Sturm sequences (8)-(9). To avoid this in double precision IEEE arithmetics it is sufficient to change these zeros to very small machine numbers. In our implementation of Godunov's algorithms it was sufficient to change elements of the main diagonal to $\epsilon_{min}/\epsilon_{mach}$, where ϵ_{min} is the smallest machine representable number and ϵ_{mach} is unit roundoff in IEEE double precision arithmetics.

Godunov's method is a direct method and due to the rounding errors in finite precision theoretical error bound for the eigenvectors computed according to the Godunov's method [8]:

$$\|(G - \mu_k I)u_k\|_2 \leq 13\sqrt{3}\,\epsilon_{mach}\,\|G\|_2\,\|u_k\|_2$$

can not be achieved. At the same time two-sided Strum sequence computations are susceptible to division by zero and overflow errors, while collinear and almost collinear eigenvectors of closely clustered and computationally coincident eigenvalues are not reorthogonalized. As a result in empirical studies residuals of Godunov's vectors appear inferior to those of the eigenvectors computed by Inverse Iteration algorithm used in the LAPACK. Godunov–Inverse Iteration uses Godunov's eigenvector u_k corresponding to an eigenvalue $\mu_k \in (\alpha_k, \beta_k)$ as an extremely accurate starting vector in a one- or two- step Inverse Iteration with selective reorthogonalization. On each step of the Godunov–Inverse Iteration the following tridiagonal linear system is solved:

$$(G - \beta_k I)x = u_k,$$

followed by Modified Gram–Schmidt reorthogonalization of the computed vector x against previous vectors that correspond to eigenvalues close or coincident with μ_k. Inverse Iteration may break down when very accurate eigenvalue approximations μ_k are used as shifts, because shifted iteration matrix $G - \mu_k I$ in this case is nearly singular. To avoid this, small perturbations are usually introduced into the shift μ_k to assure convergence to the corresponding Ritz vectors. But even small arbitrary deviations of the Ritz values from exact eigenvalues may produce significant deviations of Ritz vectors from the actual eigenvectors. We solve this problem by using either left or right-hand bound α_k or β_k of the eigenvalue interval $(\alpha_i, \beta_i) \ni \mu_i$, $i = 1, \ldots, n$ found by the bisection algorithm (either Sturm based [8] or inertia-based [5] versions of the bisection algorithm) as accurate shifts that are guaranteed to be within the error bounds (7). We use Wilkinson's stopping criteria for a nonnormalized eigenvector approximation x_k [2] $\|x_k\|_\infty \geq 2^t/100n$ to verify that convergence is achieved. In most cases convergence is achieved after one step of Inverse Iteration.

The overall computational scheme that we use to find singular vector decomposition of a real rectangular or a real bidiagonal matrix using Godunov-Inverse Iteration algorithm can be formalized as follows:

- If the original matrix is not in bidiagonal form find orthogonal transformations P and Q such that nonzero part of the matrix P^*AQ is a square bidiagonal matrix $D \in R^{n \times n}$.

- Determine n smallest machine representable intervals (α_k, β_k), $k = n+1, n+2, \ldots, 2n$ that contain n largest eigenvalues $\lambda_{n+1}, \lambda_{n+2}, \ldots, \lambda_{2n}$ of the Golub-Kahan matrix G, $\dim(G) = 2n \times 2n$. Matrix G should not be formed explicitly.

- Compute Godunov's left and right-hand Sturm sequences for the left and right bounds of the eigenintervals α_k and β_k, $k = n+1, n+2, \ldots, 2n$ respectively.

- Combine left and right Sturm sequences into a two-sided Sturm sequence and use it to recursively determine Godunov eigenvectors corresponding to the eigenvalues $\lambda_{n+1}, \lambda_{n+2}, \ldots, \lambda_{2n}$.

- Run one or two steps of the Inverse Iteration with reorthogonalization with Godunov's vectors as starting vectors to improve Godunov's eigenvectors. Use α_k or β_k instead of λ_k as Inverse Iteration shifts to avoid iteration breakdown.

- Form left singular vectors of the bidiagonal matrix D from the odd components of the iteratively improved Godunov's eigenvectors and right singular vectors from the even components of the same eigenvectors.

- If the original matrix was not bidiagonal apply orthogonal transformations P and Q^* to the matrices of left and right singular vectors of the matrix D respectively to obtain left and right singular vectors of the original matrix.

5   Experimental results

We implemented and tested Godunov's version of the bisection method which uses one-sided Sturm sequences, Godunov's method and Godunov–Inverse Iteration, which use two-sided Sturm sequences, and Inverse Iteration with random starting vectors (our implementation of the LAPACK procedure xSTEIN [10]) in ANSI C (GNU C compiler version 2.96) in IEEE double precision and tested these programs on an Intel® Xeon™ CPU 1500 MHz processor. To make a fair comparison we compute eigenvalue approximations only once and use these eigenvalues (or corresponding eigenintervals in the Godunov's routines) to compute eigenvectors using three different eigenvector methods, while in both Inverse Iteration implementations we use the same direct solver for systems of linear algebraic equations with tridiagonal symmetric matrices. Matrices $A_1 - A_4$ in the four test examples below were borrowed from [8] to illustrate results of our implementation of the Godunov's bisection method (Table 1), and to compare Godunov's method, Godunov-Inverse Iteration and Inverse Iteration with random uniform starting vectors (Table 2). By guaranteed accuracy of the computed singular values for each of the matrices $A_1 - A_4$ in the Table 1 we denote the size of the largest eigeninterval computed for the corresponding matrix. We used these values to compute corresponding singular vectors. We report residual errors and deviation from orthogonality for these singular vectors in the Table 2. We can see that residual errors and deviation from orthogonality in the singular vectors computed by Godunov's method were unacceptable. Singular vectors computed by the Godunov-Inverse Iteration in one step satisfied original problem to slightly higher accuracy than Inverse Iteration, which required tree to five iteration steps for convergence. Singular vectors computed by the Inverse Iteration were closer to orthonormal basis than singular vectors computed by the Gogunov-Inverse Iteration, but at the cost of extra iteration and reorthogonalization steps.

Test problem 1. $U^T A_1 V$, $\dim(A_1) = n \times n$, $n = 1000$.

$$A_1 = \begin{pmatrix} 1 & 10 & & & \\ & \ddots & \ddots & & \\ & & 1 & 10 & \\ & & & 1 \end{pmatrix}$$

Test problem 2. $U^T A_2 V, \ \dim(A_2) = n \times n, \ n = 1000.$

$$A_2 = \begin{pmatrix} 0.01 & 900 & & & \\ & \ddots & \ddots & & \\ & & 0.01 & 900 & \\ & & & 0.01 \end{pmatrix},$$

Test problem 3. $U^T A_3 V, \ \dim(A_3) = n \times n, \ n = 1000.$

$$A_3 = \begin{pmatrix} 0.5 & 0.5 & & & \\ & \ddots & \ddots & & \\ & & 0.5 & 0.5 & \\ & & & 0.5 \end{pmatrix},$$

Singular values of the matrix A_3 are the roots of the Chebyshev polynomials of second kind, analytical formula for which has the following form [8]:

$$\sigma_i = \frac{\cos(n-i)\,\pi}{2n+1}, \ i = 0, 1, \dots, n-1.$$

Test problem 4. $U^T A_4 V, \ \dim(A_4) = n \times n, \ n = 1000.$

$$A_4 = \begin{pmatrix} d_1 & b_1 & & & \\ & \ddots & \ddots & & \\ & & d_{n-1} & b_{n-1} & \\ & & & d_n \end{pmatrix},$$

Main diagonal: $d_i = (i+1)/\sqrt{((2i+1)(2i+3))}, \ i = 0, 2, \dots, 2n-2$, Co-diagonal: $b_i = (i+1)/\sqrt{((2i+1)(2i+3))}, \ i = 1, 3, \dots, 2n-3$. Singular values of this matrix are the orthonormal Legendre polynomials [8].

6 Conclusions

Singular value decomposition of bidiagonal matrices is equivalent to the eigenvalue problem with symmetric tridiagonal matrix with main zero diagonal, known as

Table 1. *Guaranteed accuracy of singular values computed by the Sturm-sequence based bisection method for the matrices from the test problems 1-4.*

matrix	$\max\limits_{1\leq i\leq n}\left([x_i,y_i]\ni\sigma_i\right)$	σ_{max}	σ_{min}
A_1	$2.66e-15$	$1.099995514634513e+01$	$9.3387812555515026e-21$
A_2	$2.84e-13$	$9.0000999995065263e+02$	$1.1049609838450875e-20$
A_3	$2.77e-16$	$9.9999876753247885e-01$	$7.8500557994265214e-04$
A_4	$2.77e-16$	$9.9999927746317030e-01$	$7.8520175772144713e-04$

Table 2. *Residual errors and deviation from the orthonormal basis of the singular vectors computed for the matrices from the test problems 1-4.*

matrix	method	$\|A_kV-U\Sigma\|_\infty$	$\|V^TV-I\|_\infty$	$\|U^TU-I\|_\infty$
A_1	Godunov	$9.04e-01$	$1.00e+00$	$6.56e-10$
	Inverse Iteration	$1.97e-15$	$9.68e-15$	$9.66e-15$
	Godunov Inverse Iteration	$1.66e-15$	$1.60e-12$	$1.60e-12$
A_2	Godunov	$9.99e-01$	$1.00e+00$	$4.43e-06$
	Inverse Iteration	$1.94e-15$	$2.68e-15$	$2.54e-15$
	Godunov Inverse Iteration	$1.91e-15$	$7.97e-09$	$7.97e-09$
A_3	Godunov	$1.45e-11$	$3.31e-10$	$3.32e-10$
	Inverse Iteration	$1.64e-15$	$1.02e-14$	$1.16e-14$
	Godunov Inverse Iteration	$1.50e-15$	$4.08e-13$	$4.08e-13$
A_4	Godunov	$6.14e-13$	$1.63e-10$	$1.63e-10$
	Inverse Iteration	$1.54e-15$	$5.25e-15$	$5.17e-15$
	Godunov Inverse Iteration	$1.49e-15$	$3.18e-13$	$3.18e-13$

Golub-Kahan form. This problem can be solved fast and efficiently by an interval version of the bisection method followed by Godunov-Inverse Iteration algorithm – a hybrid method based on the Godunov's two-sided Sturm sequence method and Inverse Iteration. It uses Godunov's vectors as starting vectors in the Inverse Iteration which have nontrivial component in the direction of the desired solution. To ensure that Godunov-Inverse Iteration does not break down we use either end of the computed eigenintervals rather than the centers of these intervals as the shifts in the Inverse Iteration step. Typically Godunov-Inverse Iteration converges to desired accuracy in just one step. Eigenvectors and singular vectors computed by the original Godunov's method suffer from orthogonality loss in the cases of computationally coincident or closely clustered eigenvalues. We use selective reorthogonalization of such vectors, an as a result obtain very accurate results in just one step in comparison with Inverse Iteration, which, although deliveres slightly more accurate results requires three to six iteration steps to convergence. High accuracy and low complexity make Godunov-Inverse Iteration a promising method for large scale eigenvector and singular vector computations.

Bibliography

[1] S. K. Godunov, A. G. Antonov, O. P. Kiriljuk, and V. I. Kostin. *Guaranteed accuracy in numerical linear algebra.* Kluwer Academic Publishers Group, Dordrecht, 1993. Translated and revised from the 1988 Russian original.

[2] J. H. Wilkinson. *The Algebraic Eigenvalue Problem.* Oxford University Press, 1965.

[3] Beresford N. Parlett and Inderjit S. Dhillon. Fernando's solution to Wilkinson's problem: an application of double factorization. Preprint submitted to Elsevier Science, 1996.

[4] S. K. Godunov. *Modern aspectsSingof linear algebra.* Nauchnaya Kniga, Novosibirsk, 1997. In Russian.

[5] K. V. Fernando. Accurately counting singular values of bidiagonal matrices and eigenvalues of skew-symmetric tridiagonal matrices. *SIAM Journal on Matrix Analysis and Applications*, 20(2):373–399, 1998.

[6] G. W. Stewart. On the early history of the singular value decomposition. *SIAM Review*, 35(4):551–566, 1993.

[7] G. Golub and W. Kahan. Calculating the singular values and pseudo-inverse of a matrix. *SIAM Journal on Numerical Analysis*, 2:205–224, 1965.

[8] S. K. Godunov, A. G. Antonov, O. P. Kiriljuk, and V. I. Kostin. *Guaranteed Accuracy in the Solution of SLAE in Euclidean Spaces.* Nauka, Novosibirsk, 1988. In Russian.

[9] Gene H. Golub and Charles F. Van Loan. *Matrix Computations.* The Johns Hopkins University Press, third edition, 1996.

[10] E. Anderson, Z. Bai, C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A McKenney, S. Ostrouchov, and D. Sorensen. *LAPACK Users' Guide.* SIAM, Philadelphia, second edition, 1995.